

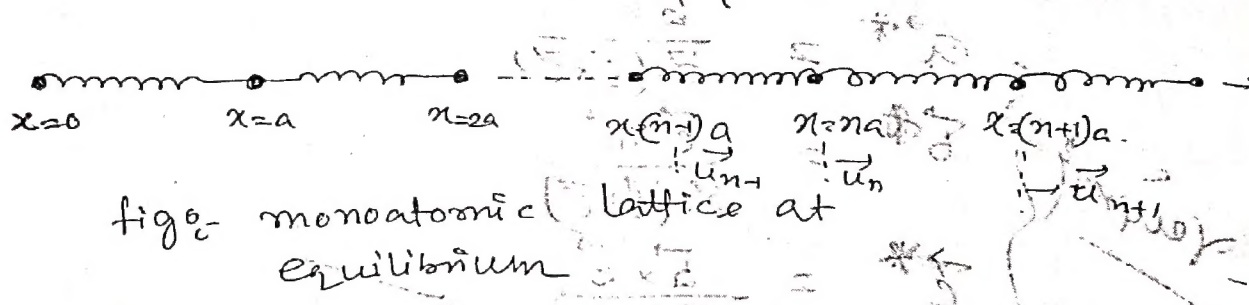
Unit-2 (Solid state)

(i) Find the dispersion relation of monoatomic lattice vibration.

(ii) Draw Dispersion graph for monoatomic lattice vibration.

→ (i) we consider a vibrating linear monoatomic lattice consist of atoms of mass ' m ' and spacing ' a ' (lattice constant).

Let, the bond between two successive atom behave as ideal spring. At equilibrium the atoms will be situated at distance ' a ' w.r to each other, from the origin the distance of $(n-1)$ th, n th, $(n+1)$ th, atom along x -axis is $(n-1)a$, na , $(n+1)a$ respectively,



Due to external force the displacement of n th of atom is u_n . Displacement of $(n-1)$ th atom is u_{n-1} and displacement of $(n+1)$ th atom is u_{n+1} .

The net force on the n th atom,

$$F_n = -\beta(u_n - u_{n-1}) - \beta(u_n - u_{n+1})$$

where, β = Spring const.
$$= \beta(u_{n+1} + u_{n-1} - 2u_n)$$

$$\Rightarrow m \frac{d^2 u_n}{dt^2} = \beta(u_{n+1} + u_{n-1} - 2u_n) \quad \text{--- (1)}$$

Let, the solⁿ of eqⁿ (1)

$$u_n = u_0 e^{i(\omega t - kx)}$$

$$u_n = u_0 e^{i(\omega t - kna)}$$

$$u_n = u_0 e^{i\left\{\frac{1}{2}\omega t - k(n-1)a\right\}}$$

$$\therefore u_{n-1} = u_0 e^{i\left\{\omega t - k(n+1)a\right\}}$$

$$u_{n+1} = u_0 e^{i\left\{\omega t - k(n+1)a\right\}}$$

$$\frac{d^2 u_n}{dt^2} = -\omega^2 u_0 e^{i(\omega t - kna)}$$

From eqⁿ (1),

$$-m\omega^2 u_0 e^{i(\omega t - kna)} = \beta \left[u_0 e^{i\left\{\omega t - k(n+1)a\right\}} + u_0 e^{i\left\{\omega t - k(n-1)a\right\}} - 2u_0 e^{i(\omega t - kna)} \right]$$

$$\Rightarrow -m\omega^2 u_0 e^{i(\omega t - kna)} = \beta \left[u_0 e^{i(\omega t - kna)} e^{-ika} + u_0 e^{i(\omega t - kna)} e^{ika} - 2u_0 e^{i(\omega t - kna)} \right]$$

$$= \beta u_0 e^{i(\omega t - kna)} \left[e^{-ika} + e^{ika} - 2 \right]$$

$$\Rightarrow m\omega^2 = \beta [2 - 2\cos ka]$$

$$\Rightarrow \omega^2 = \frac{2\beta}{m} \left[2 \sin^2 \frac{ka}{2} \right]$$

$$\therefore \omega = \sqrt{\frac{4\beta}{m}} \sin \frac{ka}{2} \quad \text{where } \beta = \frac{m}{a}$$

$$\omega = \frac{2}{a} \sqrt{\frac{c}{\rho}} \sin \frac{ka}{2}$$

$\beta = \frac{c}{a}$ = longitudinal stiffness.

$$\boxed{\omega = \frac{2}{a} v_s \sin \frac{ka}{2}}$$

$$\boxed{\omega = \omega_{\max} \sin \frac{ka}{2}}$$

$$\omega_{\max} = \frac{2}{a} v_s = \sqrt{\frac{4\beta}{m}}$$

This is the dispersion relation (relation between ω and k) for 1-D mono atomic lattice.

Case-I At low frequency: λ is very high.

k is very small. $\therefore k = \frac{2\pi}{\lambda}$

$$\therefore \sin \frac{ka}{2} \approx \frac{ka}{2}$$

$$\therefore \omega = \frac{2v_s}{a} \cdot \frac{ka}{2} \Rightarrow \omega = kv_s$$

Phase velocity, $v_p = \frac{\omega}{k} = v_s$

Group velocity, $v_g = \frac{d\omega}{dk} = v_s$, $v_g = v_p$

So, at low frequency the phase and group velocity of mono-atomic lattice vibration is equal.

Case-II At high frequency:

$$\omega = \frac{2v_s}{a} \sin \frac{ka}{2}$$

Phase velocity, $v_p = \frac{\omega}{k} = \frac{2v_s}{ak} \sin \frac{ka}{2}$

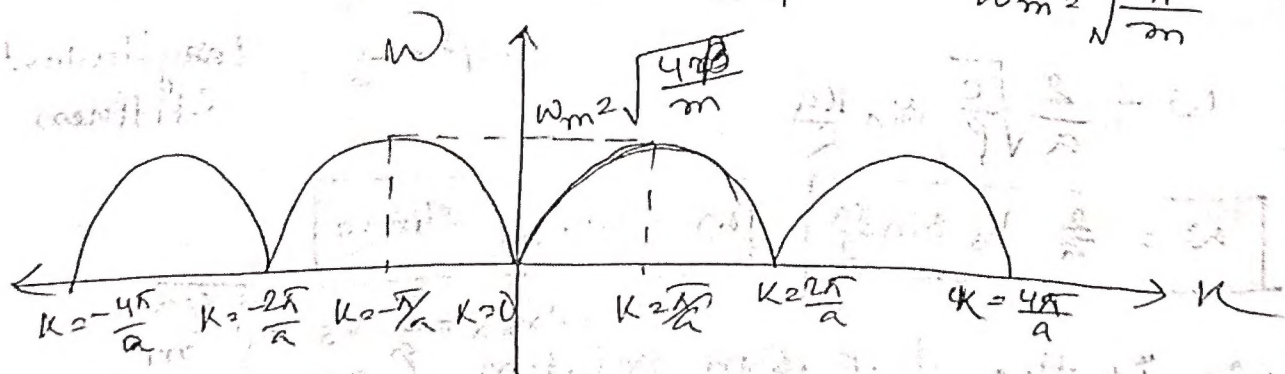
Group velocity, $v_g = \frac{d\omega}{dk} = \frac{2v_s}{a} \cos \frac{ka}{2}$
 $= v_s \cos \frac{ka}{2}$

$\therefore v_g \neq v_p$

At high frequency group velocity and phase velocity of mono-atomic lattice vibration is not equal.

(ii) Graphical representation of dispersion relation

$$\omega = \omega_m \left| \sin \frac{ka}{2} \right|, \text{ where } \omega_m = \sqrt{\frac{4\beta}{m}}$$



By plotting ω vs k graph we get a sinusoidal curve with period $\frac{2\pi}{a}$

The region in betⁿ π/a to $-\pi/a$ is known as '1st' Brillouin Zone. $(-\pi/a < k < \pi/a)$

(*) for a mono atomic lattice vibration spring const. is 0.02 N/m and mass of each atom is 1 mg . Find the maximum frequency of dispersion.

→ We know that,

$$\omega_{\max} = \sqrt{\frac{4\beta}{m}} = 2 \sqrt{\frac{2}{100 \times 10^{-3} \times 10^{-3}}}$$

$$= 2 \times 141.4$$

$$\omega_{\max} = 282.8 \text{ Hz}$$

(2) (i) what is phonon? Discuss how phonon is related to lattice vibration.

(ii) Write down the difference between phonon and photon.

→ (i) The quantum of energy in lattice vibration is called phonon. Phonon is analogous to photon in electromagnetic radiation.

The energy in lattice vibration is quantised. When an elastic wave is excited the atoms in the lattice 'n' no. of phonons are generated. The elastic mode energy can be written as,

$E_n = (n + \frac{1}{2}) \hbar \omega$, where, $\frac{\hbar \omega}{2} = \text{Zero point energy}$.
as the lattice vibration energy is quantised. so, phonon energy is also quantised.

The range of frequency of phonon is 10^4 to 10^{12} Hz . Phonon are like photons with zero spin. The phonons obey Bose-Einstein distribution.

Physically a phonon has zero momentum, but practically when a phonon interacts with proton, electron has momentum $\hbar k$. The momentum

$\hbar k$ is also known as crystal momentum.

(i) phonon

(a) phonons are quantum of lattice vibration.

(b) phonons has zero spin.

(c) Physically Phonon has zero momentum.

photon

(a) photons are quantum of EM radiation.

(b) The spin of photon is \hbar .

(c) photon has momentum $\frac{h\nu}{c}$.

(3) write down some practical evidence of phonons in lattice vibration?

$$W_{\max} = 2 \frac{2\nu_s}{\lambda}$$

$$\Rightarrow W_{\max} = \frac{2}{4.85 \times 10^8} \times 1.08 \times 10^4 \text{ s}^{-1}$$

$$\Rightarrow W_{\max} = 0.445 \times 10^{12} \text{ Hz}$$

$$W_{\max} = \sqrt{\frac{4\beta}{m}} = 0.445 \times 10^{12}$$

$$\Rightarrow 2 \sqrt{\frac{\beta}{6.81 \times 10^{-26}}} = 0.445 \times 10^{12}$$

$$\Rightarrow \frac{\sqrt{\beta \times 10^{13}}}{2.609} = 0.2225 \times 10^{12}$$

$$\Rightarrow \sqrt{\beta} = 0.580 \times 10^{-1}$$

$$\Rightarrow \beta = 0.0580$$

$$\Rightarrow \beta = 0.003369$$

$$\vec{A} = \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix}$$

$$\vec{B} = \frac{1}{\sqrt{2}} \begin{pmatrix} \hat{x} \\ -\hat{y} \end{pmatrix}$$

$$\vec{C} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\hat{x} \\ \hat{y} \end{pmatrix}$$

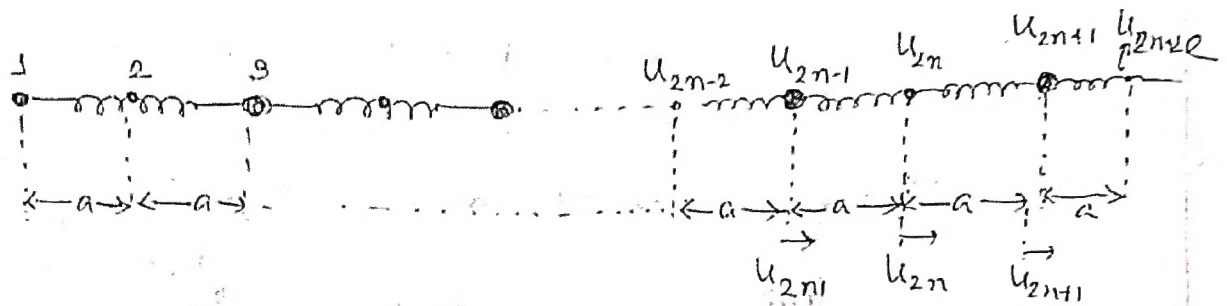
$$\vec{D} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\hat{x} \\ -\hat{y} \end{pmatrix}$$

(i) Find the dispersion relation of linear diatomic molecule.

(ii) Draw ω vs k graph for linear diatomic vibration.

(iii) Discuss Acoustic Branch and the optical branch of linear diatomic lattice.

→ (i) We consider a linear diatomic molecule consist of two different atoms of mass M and m , ($M > m$). The nearest neighbour distance or the separation between two successive atoms is a . The spring constant between the atoms is β .



The equation of motion of the atom having mass M .

$$M \frac{d^2 u_{2n-1}}{dt^2} = \beta (u_{2n} - 2u_{2n-1} + u_{2n-2}) \rightarrow (i)$$

The equation of motion for the atom having mass, m .

$$m \frac{d^2 u_{2n}}{dt^2} = \beta (u_{2n+1} - 2u_{2n} + u_{2n-1}) \rightarrow (ii)$$

The general solⁿ of eqⁿ (i)

$$u_{2n-1} = B e^{-i \{ K(2n-1)a - \omega t \}} \rightarrow (iii)$$

and general solⁿ of eqⁿ (ii),

$$u_{2n} = A e^{i \{ K 2na - \omega t \}} \rightarrow (iv)$$

Here,
A, B are
arbitrary
const.

using eqn (iii) and (iv) in eqn (i) and (ii) we get,

$$(-2\beta \cos Ka) A + (2\beta - \omega^2 M) B = 0 \quad \text{--- (v)}$$

$$(2\beta - \omega^2 m) A - (2\beta \cos Ka) B = 0 \quad \text{--- (vi)}$$

The eqn (v) and (vi) has non-zero solⁿ ($A \neq 0, B \neq 0$) if the determinant of the co-efficients is equal to zero.

$$\begin{vmatrix} -2\beta \cos Ka & 2\beta - \omega^2 M \\ 2\beta - \omega^2 m & -2\beta \cos Ka \end{vmatrix} = 0$$

$$\Rightarrow 4\beta^2 \cos^2 Ka - 4\beta^2 + 2\beta \omega^2 M + 2\beta \omega^2 m - \omega^4 Mm = 0$$

$$\Rightarrow Mm\omega^4 - 2\beta\omega^2(M+m) + 4\beta^2(1 - \cos^2 Ka) = 0 \quad \text{--- (vii)}$$

where, eqn (vii) is a quadratic eqn of ω^2 ,

$$\omega^2 = \frac{+2\beta(M+m) \pm \sqrt{4\beta^2(M+m)^2 - 16Mm\beta^2(1 - \cos^2 Ka)}}{2Mm}$$

$$= \frac{2\beta(M+m) \pm 2\beta \sqrt{(M+m)^2 - 4Mm + 4Mm \cos^2 Ka}}{2Mm}$$

$$= \beta \left(\frac{1}{M} + \frac{1}{m} \right) \pm \beta \sqrt{\frac{(M-m)^2 + 4Mm \cos^2 Ka}{(Mm)^2}}$$

$$\boxed{\omega^2 = \beta \left(\frac{1}{M} + \frac{1}{m} \right) \pm \beta \sqrt{\left(\frac{1}{M} - \frac{1}{m} \right)^2 + \frac{4 \cos^2 Ka}{Mm}}}$$

This is the dispersion relation for di-atomic linear lattice.

(iii) The acoustic branches -

The dispersion relation corresponding to acoustic branch is given by,

$$\omega_-^2 = \beta \left(\frac{1}{M} + \frac{1}{m} \right) - \beta \sqrt{\left(\frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4 \cos^2 Ka}{Mm}}$$

$$\Rightarrow \omega_-^2 = \beta \left(\frac{1}{M} + \frac{1}{m} \right) - \beta \sqrt{\left(\frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4 \sin^2 Ka}{Mm}}$$

When, $K=0$, $\omega_-^2 = 0$.

$\therefore \omega_- = 0$ at $K=0$.

When, $K = \pm \frac{\pi}{2a}$;

$$\omega_-^2 = \beta \left(\frac{1}{M} + \frac{1}{m} \right) - \beta \sqrt{\left(\frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4}{Mm}}$$

$$= \beta \left(\frac{1}{M} + \frac{1}{m} \right) - \beta \sqrt{\left(\frac{1}{m} - \frac{1}{M} \right)^2}$$

$$= \beta \left(\frac{1}{M} + \frac{1}{m} \right) - \beta \left(\frac{1}{m} - \frac{1}{M} \right) \quad ; M > m$$

$$\frac{1}{M} < \frac{1}{m}$$

$$\Rightarrow \omega_-^2 = \frac{2\beta}{M}$$

$$\Rightarrow \omega_- = \sqrt{\frac{2\beta}{M}}$$

The optical branches

The dispersion relation for optical branch is given by,

$$\omega_+^2 = \beta \left(\frac{1}{M} + \frac{1}{m} \right) + \beta \left[\left(\frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4 \sin^2 Ka}{Mm} \right]^{\frac{1}{2}}$$

When, $K=0$,

$$\omega_+^2 = \beta \left(\frac{1}{M} + \frac{1}{m} \right) + \beta \left(\frac{1}{M} + \frac{1}{m} \right)$$

$$= 2\beta \left(\frac{m+M}{Mm} \right)$$

$$\therefore \omega_+ = \sqrt{2\beta \left(\frac{M+m}{Mm} \right)}$$

when, $K = \pm \frac{\pi}{2a}$,

$$\omega_+^2 = \beta \left(\frac{1}{M} + \frac{1}{m} \right) + \beta \left[\left(\frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4}{Mm} \right]^{\frac{1}{2}}$$

$$= \beta \left(\frac{1}{M} + \frac{1}{m} \right) + \beta \left[\left(\frac{1}{m} - \frac{1}{M} \right)^2 \right]^{\frac{1}{2}}$$

$$\omega_+^2 = \frac{2\beta}{m}$$

$$\therefore \omega_+ = \sqrt{\frac{2\beta}{m}}$$

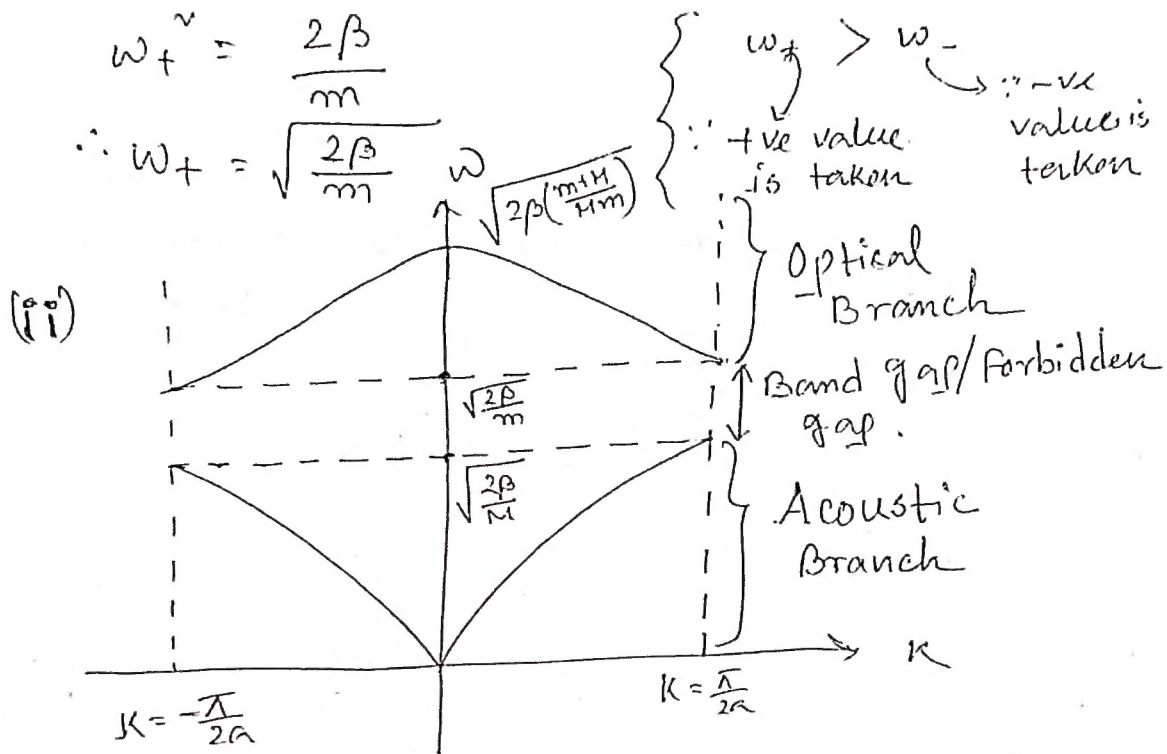


Fig:- Dispersion Curve/ ω vs K curve for 1-D diatomic lattice ($M > m$).

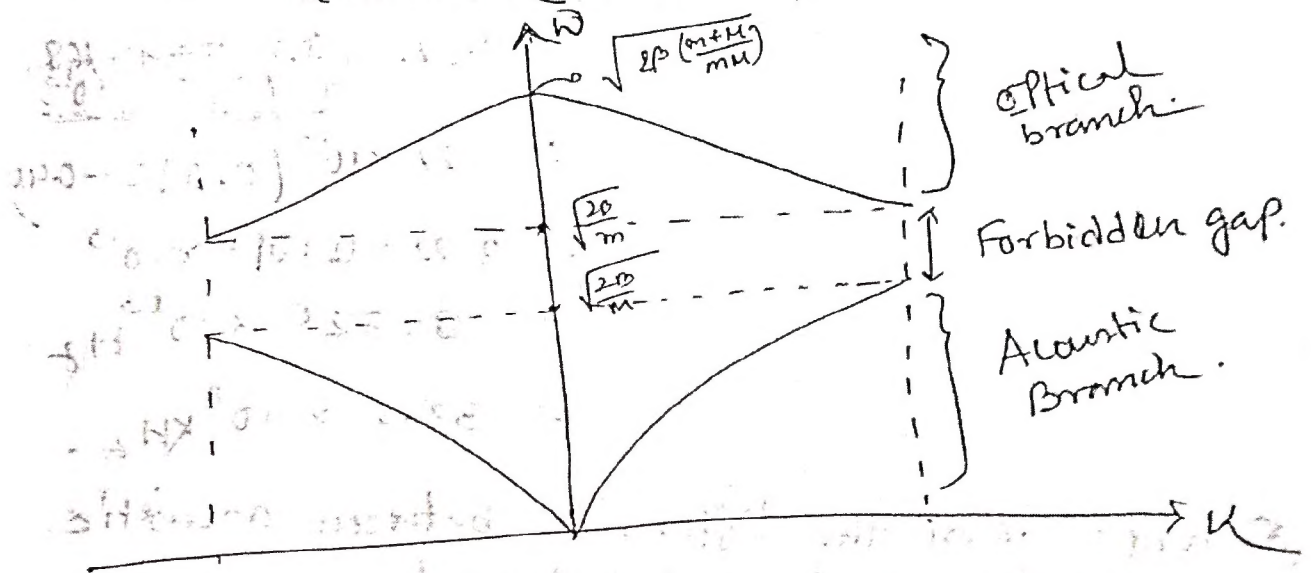
(*) (i) What do you mean by Forbidden gap.

(ii) Explain Di-atomic linear lattice can be act as mechanical band reject filter.

(i) \rightarrow For the lattice vibration of Diatomic for linear lattice there are two branches of dispersion, they are - (i) optical branch (ii) acoustic branch.

The range of frequency inbetween upper limit of acoustic branch and lower limit of optical branch is known as forbidden frequency gap, the lattice cannot vibrate with this range of frequency.

this behaviour of diatomic linear lattice is similar to band reject filter of electronic this is why diatomic linear lattice can be act as mechanical band reject filter.



$$\text{Forbidden gap } \Delta = \sqrt{\frac{2\beta}{m}} - \sqrt{\frac{2\beta}{M}}$$

$$\Delta = \sqrt{2\beta} \left(\frac{1}{\sqrt{m}} - \frac{1}{\sqrt{M}} \right)$$

$$\text{In linear frequency, } \Delta = \frac{\sqrt{2\beta}}{2\pi} \left(\frac{1}{\sqrt{m}} - \frac{1}{\sqrt{M}} \right)$$

for Mono-atomic lattice; $m = M$

$$\boxed{\Delta = 0}$$

(*) For NaCl crystal, find forbidden gap, frequency in KHz, if force const. of NaCl is 205 N/m

→ Force const. $\beta = 205 \text{ N/m}$

$m = 23, M = \text{Cl} = 35.5 \text{ amu}$
Na amu

Forbidden gap for linear form

$$\Delta = \frac{\sqrt{2\beta}}{2\pi} \left(\frac{1}{\sqrt{23}} - \frac{1}{\sqrt{35.5}} \right)$$

$$= 3.22 \left(\frac{1}{\sqrt{23}} - \frac{1}{\sqrt{35.5}} \right)$$

$$= 3.22 \times 10^{13} (0.512 - 0.41)$$

$$= 3.22 \times 0.1011 \times 10^{13}$$

$$= 0.325 \times 10^{13} \text{ Hz}$$

$$= 32.5 \times 10^8 \text{ KHz}$$

(*) Write down the difference between acoustic branch and optical branch.

→ acoustic | optical

(i) In acoustic branch the frequency of lattice vibration is maximum at

$$k = \pm \frac{\pi}{2a}$$

(i) In optical branch the frequency of lattice vibration is maximum at

$$k = 0$$

(ii) In acoustic branch the frequency of lattice vibration is minimum at $k = 0$.

(ii) In optical the frequency is minima at $k = \pm \frac{\pi}{2a}$

(iii) at $K=0$ the amplitude of vibration is in same phase for both the atom.

(iii) at $K=0$ the amplitude of vibration is in out of phase for both the atom.

(iv) at $K = \pm \frac{\pi}{2a}$, the smaller atom is at rest at the bigger atom is vibrating

(iv) at $K = \pm \frac{\pi}{2a}$, the smaller atom is vibrating & the bigger atom is at rest.

Specific heat of solid:-

① (i) Proof of Dulong-Petit's law of specific heat.

OR

Proof of classical theory of specific heat of solid.

→ (i) Write down the limitations of Dulong-Petit's law of specific heat.

→ (i) classical theory assumed that each atom in a crystal behave as 3-D simple harmonic vibrator.

Let, there are N no's of atoms in a solid. For each atom, the no. of degrees of freedom is equal to '6'. (3 translational and 3 rotational) from equipartition theorem, KE per Degree of freedom = $\frac{1}{2} kT$, $k = \text{Boltzmann's const.}$

KE for 1 atom = $6 \times \frac{1}{2} kT = 3kT$. T = Temp. in Kelvin.

For whole solid the Internal energy

$$U = N \cdot 3kT$$

$$= 3NkT; \quad \text{for 1 mole, } N = N_A$$

$$\boxed{U = 3RT} \quad \text{for 1 mole.} \quad [kN_A = R]$$

Molar specific heat of solid at
const. volume, $C_V = \left(\frac{\partial U}{\partial T} \right)_V$

$$\boxed{C_V = 3R}$$

this is the expression for specific heat of
solid, according to Dulong-Peitt's
theory.

(ii) Limitations :-

(a) Dulong-Peitt's law is only valid
in high temp.

(b) There are many solids with
high melting point whose specific
heat less than $3R$.

(c) there are many metals with
low melting point, has specific heat
greater than $3R$.

(d) From Expt. result, the specific heat
of solid varies with temp. It is
not const.

(*) Derive an expression for specific heat capacity of solid according to Einstein theory.
 → From Einstein theory, the crystal atoms behave as harmonic oscillator and vibrates independently with frequency ω_0 , the atom's can only exchange discrete energy value such that,

$$E_n = n\hbar\omega_0; \quad n=0, 1, 2, 3, \dots$$

the no. of atoms at energy E_n is given by $N_n \propto e^{-E_n/KT}$, where K = Boltzmann const.

$$N_n = N_0 e^{-E_n/KT}, \quad N_0 = \text{Number of atom}$$

Average energy per oscillator; with energy $E=0$.

$$\bar{E} = \frac{\text{Total energy}}{\text{Total no. of atoms}}$$

$$= \frac{0 \times N_0 + E N_1 + 2E N_2 + \dots}{N_0 + N_1 + N_2 + \dots}$$

$$= \frac{0 \times N_0 + E_0 N_0 e^{-\frac{E}{KT}} + 2E N_0 e^{-\frac{2E}{KT}} + \dots}{N_0 + N_0 e^{-\frac{E}{KT}} + N_0 e^{-\frac{2E}{KT}} + \dots}$$

$$= \hbar\omega_0 \frac{e^x + 2e^{2x} + 3e^{3x} + \dots}{1 + e^x + e^{2x} + e^{3x} + \dots}$$

$$= \hbar\omega_0 \frac{d}{dx} \left[\ln(1 + e^x + e^{2x} + e^{3x} + \dots) \right] \left[x = -\frac{\hbar\omega_0}{KT} \right]$$

$$= \hbar\omega_0 \frac{d}{dx} \left\{ \ln \left(\frac{1}{1 - e^x} \right) \right\}$$

$$= \hbar\omega_0 (-1) \frac{1}{1 - e^x} (-e^x) = \hbar\omega_0 \frac{e^x}{1 - e^x}$$

$$= \frac{\hbar \omega_0}{e^{\frac{\hbar \omega_0}{kT}} - 1}$$

the total internal energy of the solid,

$U = 3N\bar{E}$, for each atom there are 3 oscillators.

$$U = \frac{3N\hbar\omega_0}{e^{\frac{\hbar\omega_0}{kT}} - 1} \quad \text{--- (i)}$$

Specific heat of solid at const. volume,

$$C_V = \left(\frac{\partial U}{\partial T} \right)_V$$

$$C_V = 3N\hbar\omega_0 \left(\frac{1}{T} \right) \left(e^{\frac{\hbar\omega_0}{kT}} - 1 \right)^{-2} e^{\frac{\hbar\omega_0}{kT} \cdot \frac{\hbar\omega_0}{kT}}$$

$$C_V = 3Nk \left(\frac{\hbar\omega_0}{kT} \right)^2 \left(e^{\frac{\hbar\omega_0}{kT}} - 1 \right)^{-2} e^{\frac{\hbar\omega_0}{kT}}$$

$$= 3R \left(\frac{\Theta_E}{T} \right)^2 \left(e^{\frac{\Theta_E}{T}} - 1 \right)^{-2} e^{\frac{\Theta_E}{T}}$$

$$= 3R \left(\frac{\Theta_E}{T} \right)^2 \frac{e^{\frac{\Theta_E}{T}}}{\left\{ e^{\frac{\Theta_E}{T}} - 1 \right\}^2}$$

* Case - I

for high temp:-

$$T \gg \Theta_E$$

$$e^{\frac{\Theta_E}{T}} = 1 + \frac{\Theta_E}{T} + \text{H.O.T.}$$

as, $\frac{\Theta_E}{T} \ll 1$, we can neglect H.O.T. terms.

from Einstein specific heat eqn.

$$C_V = 3R \left(\frac{\Theta_E}{T} \right)^2 \frac{1 + \frac{\Theta_E}{T}}{\left(1 + \frac{\Theta_E}{T} - 1 \right)^2}$$

$$= 3R \left(1 + \frac{\Theta_E}{T} \right)$$

$$C_V \approx 3R$$

i.e. at high temp. Einstein specific heat for solid is equal to the Dulong Petit's value of specific heat.

case - II at low Temp. $T \ll \Theta_E$

$$\text{as } T \ll \Theta_E$$

$$\frac{\Theta_E}{T} \gg 1$$

$$\text{hence } e^{\frac{\Theta_E}{T}} \gg 1$$

$$\frac{\Theta_E}{T} \gg 1 \Rightarrow e^{\frac{\Theta_E}{T}} \approx e^{\frac{\Theta_E}{T}}$$

from Einstein specific heat eqn,

$$C_V = 3R \left(\frac{\Theta_E}{T} \right)^2 \frac{e^{\frac{\Theta_E}{T}}}{e^{2\frac{\Theta_E}{T}}}$$

$$C_V = 3R \left(\frac{\Theta_E}{T} \right)^2 e^{-\frac{\Theta_E}{T}}$$

from this eqn specific heat approaches to zero as the Temp. T approaches to zero, which does not obey the experimental law of

specific heat at low temp. From heat time data, we get, specific heat of solid varies T^3 at low temp.

⑤ Explain why Einstein theory is not capable of giving correct behaviour of specific heat at low Temp.

→ The reason for the disagreement of the Einstein theory of specific heat with experimental result, due to over simplified model used, in which all the atoms, of the solid, vibrating independently with unique frequency ω_0 . But in practical the atom's coupled together can vibrate with a range of frequency rather than just a single frequency ω_0 .

⑥ Explain Debye model of specific heat of solid

→ Debye pointed out that the source of error in Einstein theory of specific heat lies in the consideration that all the oscillator's vibrates with const. frequency ω_0 . Debye considered that the atom's of the solid coupled together and vibrates with a range of frequency. Once the density function $\rho(\omega)$ of the frequency of vibration is known we can easily calculate, the total internal energy of the solid

Total internal energy of the solid,

$$E = \int \bar{E}(\nu) g(\nu) d\nu \quad \text{--- (i)}$$

all allowed frequency

where,

$\bar{E}(\nu)$ = average energy per oscillator

The no. of oscillator having energy $h\nu$ is proportional to $e^{-\frac{h\nu}{kT}}$.

The average KE, $\bar{E} = \frac{N_0 \times 0 + N_1 h\nu + N_2 2h\nu + \dots}{N_0 + N_1 + N_2 + \dots}$

$$= \frac{N_0 (h\nu e^{-\frac{h\nu}{kT}} + 2h\nu e^{-\frac{2h\nu}{kT}} + \dots)}{N_0 (1 + e^{-\frac{h\nu}{kT}} + e^{-\frac{2h\nu}{kT}} + \dots)}$$

$$= h\nu \frac{(e^{-\frac{h\nu}{kT}} + 2e^{-\frac{2h\nu}{kT}} + 3e^{-\frac{3h\nu}{kT}} + \dots)}{(1 + e^{-\frac{h\nu}{kT}} + e^{-\frac{2h\nu}{kT}} + \dots)}$$

$$= h\nu \frac{d}{dn} \left\{ \ln (1 + e^{-\frac{h\nu}{kT}} + e^{-\frac{2h\nu}{kT}} + \dots) \right\} \quad n = -\frac{h\nu}{kT}$$

$$= h\nu \frac{d}{dn} \left\{ \ln \frac{1}{1 - e^{-n}} \right\}$$

$$= h\nu (-1)(1 - e^{-n}) (-e^{-n})$$

$$= \frac{h\nu \cdot e^{-n}}{1 - e^{-n}}$$

$$\bar{E}(\nu) = \frac{h\nu}{e^{-\frac{h\nu}{kT}} - 1} \quad \text{--- (ii)}$$

Density of state having frequency ν is given by

$$g(\nu) d\nu = 4\pi V \left(\frac{1}{V_l^3} + \frac{2}{V_t^3} \right) \nu^2 d\nu$$

where,

V_l = Longitudinal wave velocity

V_t = Transverse wave velocity

$$g(\nu) d\nu = \frac{9N}{V_0^3} \nu^2 d\nu \quad \text{--- (iii)} \quad \begin{matrix} \text{Wave velocity} \\ \text{Volume of the solid.} \end{matrix}$$

$$\nu \leq \nu_0$$

$$\nu > \nu_0$$

where, ν_0 = Debye frequency.

Using eq. (ii) and (iii) in

N = Number of atoms.

$$\begin{aligned} \text{(i), } E &= \frac{9N}{V_0^3} \int_0^{\nu_D} \frac{h\nu^3 d\nu}{e^{\frac{h\nu}{KT}} - 1} \quad \left| \begin{array}{l} \nu_D = \frac{h\nu_D}{KT} \\ \text{Let, } x = \frac{h\nu}{KT} \\ d\nu = \frac{KT}{h} dx \end{array} \right. \\ &= \frac{9N}{V_0^3} \left(\frac{KT}{h\nu_D} \right)^3 \int_0^{x_D} \frac{x^3}{e^x - 1} dx \end{aligned}$$

We can define the Debye temperature as Θ_D according to the eqn $h\nu_D = k\Theta_D$

$$\Theta_D = \frac{h\nu_D}{k} \quad \text{and} \quad x_D = \frac{\Theta_D}{T}$$

$$E = 9RT \left(\frac{T}{\Theta_D} \right)^3 \int_0^{x_D} \frac{x^3}{e^x - 1} dx$$

Case-I at high temp. $T \gg \theta_D$, hence $kT \gg \hbar \nu$

$$e^x - 1 \approx 1 + x - 1 \approx x$$

$$E = 9NkT \left(\frac{T}{\theta_D} \right)^3 \frac{2\theta_D^3}{3}$$
$$= 3NkT \left(\frac{T}{\theta_D} \right)^3 \cdot \left(\frac{\theta_D}{T} \right)^3$$

$$E = 3RT$$

$\therefore C_V = \left(\frac{\partial E}{\partial T} \right)_V = 3R$
at high temp. Debye's theory is similar to Dulong's
Petit's theory of Specific heat.

Case-II at low temp. $T \ll \theta_D$; hence,

In this case, the upper limit, $\hbar \nu_D \gg kT$
of integration, becomes infinite,
($x_D \rightarrow \infty$)

$$\therefore \int_0^{\infty} \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}$$

$$E = 9RT \left(\frac{T}{\theta_D} \right)^3 \cdot \frac{\pi^4}{15}$$

Specific heat,

$$C_V = \left(\frac{\partial E}{\partial T} \right)_V = 9R \cdot \frac{1}{\theta_D^3} \cdot 4T^3 \cdot \frac{\pi^4}{15}$$

$$\boxed{C_V \propto T^3}$$

This is known as T^3 law of specific heat.

(*) Write down the limitations of Debye's theory of specific heat?

write down the limitations of Debye's theory of specific heat?



Calculate the Debye specific heat of copper at 10K and 300K, given that the Debye characteristic frequency is 6.55×10^{12} Hz.

→ Here, Debye frequency $\nu_D = 6.55 \times 10^{12}$ Hz.
We know that, Debye temp., $\theta_D = \frac{h\nu_D}{k}$

$$\text{for, } T = 10K, \quad \theta_D = \frac{6.626 \times 10^{-34} \times 6.55 \times 10^{12}}{1.38 \times 10^{-23}}$$

$$T \ll \theta_D \quad (\text{low temp.}) \quad \theta_D = 31.49 \times 10 \\ = 314.49 \text{ K}$$

$$C_V = \frac{9 \times 4}{15} \pi^4 R \left(\frac{T}{\theta_D} \right)^3 \\ = \frac{12}{5} \times \frac{(314)^4}{10^5} \times 8.314 \times \frac{10^3}{(314.5)^3}$$

$$= 0.0626 \text{ J/K-mol}$$

for, $T = 300K$ - at high temp,
 $C_V = 3R \text{ J.K}^{-1}\text{mol}^{-1}$

$$= 3 \times 8.314 \\ = 24.942 \text{ J.K}^{-1}\text{mol}^{-1}$$

Q (i) Define Mean free time, Mean free path of electron?

(ii) Find an Expression for electric conductivity of metal?

*** (iii) Deduce, Wiedemann-Franz law?

→ In metal, there are huge no. of free electron or semi-free electron and there is collision between them due to their random motion. The distance travelled by an electron between two successive collision is known as Mean free path, and the time taken between two successive collision is known as Mean free time.

(ii) Electric conductivity :-

In presence of electric field (\vec{E}), the Drift velocity (v_d) of electron increases with time,

$$\therefore \left(\frac{\partial v_d}{\partial t} \right) = - \frac{eE}{m} \quad \rightarrow (i)$$

We consider that in a collision with the lattice the electron loses all its KE it has gained from the external electric field. And its velocity after the collision is not dependent upon the direction of motion before the collision.

for the electron lattice collision, we can write

$$\frac{dV_D}{dt} = -\frac{V_D}{\tau} \rightarrow (ii) \quad [\tau = \text{mean free time}]$$

At steady state, the acceleration of the electron will become zero.

$$\frac{dV_D}{dt} = 0$$

$$\left(\frac{\partial V_D}{\partial t} \right)_{\text{electric field}} + \left(\frac{\partial V_D}{\partial t} \right)_{\text{collision}} = 0$$

$$\Rightarrow -\frac{eE}{m} - \frac{V_D}{\tau} = 0$$

$$\Rightarrow V_D = -\frac{eE\tau}{m} \rightarrow (iii)$$

Again from ohm's law the current density

$$J = \sigma(E) \quad \sigma = \text{conductivity}$$

$$\Rightarrow -nev_D = \sigma E$$

$n = \text{no. of e}^- \text{ per unit vol.}$

$$\Rightarrow V_D = -\frac{\sigma E}{ne} \rightarrow (iv)$$

From eqⁿ (iii) and (iv)

$$\frac{eE\tau}{m} = \frac{\sigma E}{ne}$$

$$\lambda = \frac{\lambda}{v_F}$$

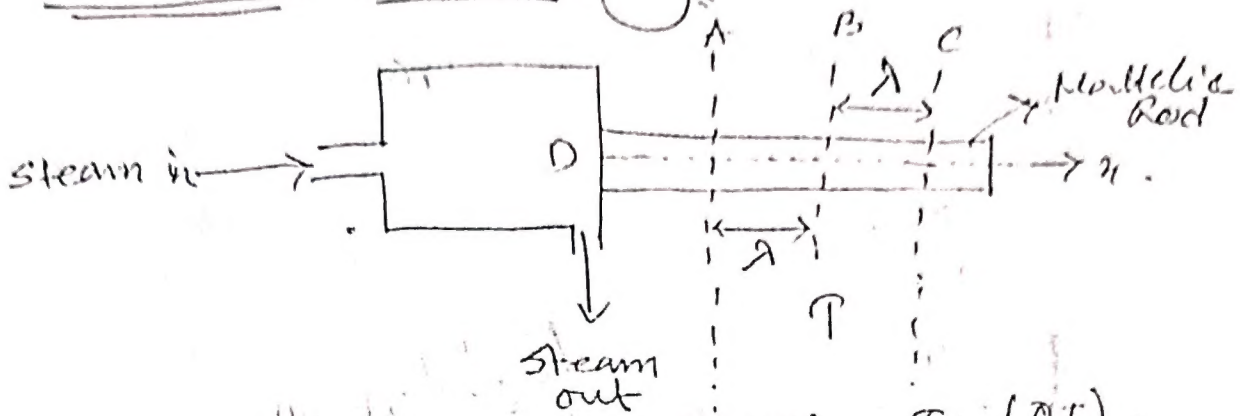
$v_F = \text{Fermi velocity}$

$$\Rightarrow \sigma = \frac{ne^2\tau}{m}$$

$$\sigma = \frac{ne^2}{m} \frac{\lambda}{v_F}$$

this is the Expression for electric conductivity for the metals.

Thermal conductivity



We consider a Rod with uniform cross-section as shown in fig. A, B, C are three layers normal to the direction of heat flow - Let, each of the layer is separated by a distance λ (Mean free path of e). The Temp. of layer A is $T + \left(\frac{dT}{dx}\right)\lambda$, $\left(\frac{dT}{dx} = \text{Temp. Gradient}\right)$ where, T is the temp. of layer B. the temp. of layer C is $T - \left(\frac{dT}{dx}\right)\lambda$. the thermal energy of electron in this layer's A, B, C is, $E + \left(\frac{dE}{dx}\right)\lambda$, E , $E - \left(\frac{dE}{dx}\right)\lambda$ respectively.

Heat energy carried by electrons through per unit cross-section area in unit time through the middle layer B, $\frac{1}{6} n e v \left(\frac{dE}{dx}\right)\lambda$

Similarly, heat energy transported through middle layer B in opposite direction, n - no of e^- Fermi vol^m
 \bar{c} - average velocity of e^-
 $-\frac{1}{6} n \bar{c} \left(\frac{\partial E}{\partial x} \right) \lambda$

Hence, net heat energy transported through Fermi cross section area in unit time,

$$= \frac{1}{6} n \bar{c} \left(\frac{\partial E}{\partial x} \right) \lambda -$$

$$\left[-\frac{1}{6} n \bar{c} \left(\frac{\partial E}{\partial x} \right) \lambda \right]$$

$$= \frac{1}{3} n \bar{c} \left(\frac{\partial E}{\partial x} \right) \lambda$$

$$= \frac{1}{3} n \bar{c} \left(\frac{\partial E}{\partial T} \right) \left(\frac{\partial T}{\partial x} \right) \lambda$$

$$= \frac{1}{3} n \bar{c} \lambda (C_v)_e \left(\frac{\partial T}{\partial x} \right)$$

$(C_v)_e$ = electric

specific

heat

$$= \sigma_T \left(\frac{\partial T}{\partial x} \right)$$

So, thermal conductivity $\sigma_T = \frac{1}{3} n \bar{c} \lambda (C_v)_e$

where,

E_F = Fermi energy

$$= \frac{1}{2} m v_F^2$$

$\bar{c} = v_F$ = average velocity / Fermi-velocity

$$\sigma_T = \frac{\pi^2}{3} \frac{n k^2 T}{m} \tau$$

this is the expression for thermal conductivity of metal.

(iii) We know that, $\sigma_T = \frac{\pi^2}{3} \cdot \frac{n k^2 T}{m} \tau$

And, electric conductivity, $\sigma = \frac{n e^2 \tau}{m}$

$$\therefore \frac{\sigma_T}{\sigma} = \frac{\pi^2}{3} \left(\frac{k}{e} \right)^2 T$$

$$\boxed{\frac{\sigma_T}{\sigma} = L T}$$

where

$$L = \frac{\pi^2}{3} \left(\frac{k}{e} \right)^2$$

$$= 2.84 \times 10^{-8} \text{ Watt}^{-1} \Omega$$

This is known as

= Lorentz Number

Wiedemann-Franz law.

(*) Define Drift velocity, mobility, Fermi velocity &

→ Drift velocity: The net velocity in a conductor due to the moving of electrons is referred to as the drift velocity of electrons (v_d)

Mobility :- Mobility of a carrier is the drift velocity per unit electric field. (μ)

Fermi velocity :- In conductor only those electrons that lie within the range kT of the Fermi level are active in the transport process. The velocity of such electron is Fermi ~~level~~ velocity.

(12)

The Fastest ones are moving at a velocity corresponding to a kinetic energy equal to the Fermi energy. This ^{velocity} ~~speed~~ is known as the Fermi ~~energy~~ velocity.